

SELF-ADAPTIVE INCREMENTAL NEWTON-RAPHSON ALGORITHMS*

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SUMMARY

Multilevel self-adaptive Newton-Raphson type strategies are developed to improve the solution efficiency of nonlinear finite element simulations of statically loaded structures. The overall strategy involves three basic levels. The first level involves preliminary solution "tunneling" via primitive operators. Secondly, the solution is constantly monitored via so-called quality/convergence/nonlinearity tests. Lastly, the third level involves self-adaptive algorithmic update procedures aimed at improving the convergence characteristics of the Newton-Raphson strategy. Numerical experiments are included to illustrate the results of the procedure.

INTRODUCTION

Finite element (FE) or difference simulations of continuum problems generally lead to nonlinear modelling equations [1,2]. Generally, such simulations must be solved by various techniques which are inherently iterative in nature. For instance, such methodologies as direct numerical integration, Newton-Raphson (NR), and modified Newton-Raphson (MNR), as well as the incremental versions of such procedures (INR, IMNR) have all been employed [2]. Since the types of nonlinearity exhibited by continuum problems are both diverse and complex, the question of the best choice of an appropriate solution algorithm inevitably arises. Note, while many alternatives are available, generally the various solution procedures may have special advantages for certain classes of problems but may exhibit poor convergence for other situations.

In this context, the ideal general purpose (GP) nonlinear FE code should have numerous algorithmic options augmented with a degree of artificial intelligence. Namely, the problem solving capability should involve a heuristically guided trial and error search in the space of possible solution via an automatically structured algorithm. Unfortunately, because of the inherent difficulties associated with code architecture and kinematic, kinetic, constitutive and boundary condition formulations, generally only one algorithmic option is usually available in GP codes. In this context, because of its wide

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applicability, most GP nonlinear FE codes employ some variant of either the straight or modified INR algorithmic procedures.

Note, while nonlinear codes present the user with far reaching capabilities, without a priori physical insight, expensive parametric studies are oftentimes necessary to insure adequate solution convergence. For instance, unless the proper load increment is employed, either poor convergence or out of balance loads are generally encountered. Incorporating heuristic programming could eliminate some of the expensive and time consuming parametric studies that are now required to determine the proper incrementation necessary for reasonable convergence.

In view of the shortcomings of the current generation of solution algorithms, this paper will consider the development of self-adaptive NR strategies for the solution of nonlinear FE or difference simulations of statically loaded structures. The main thrust will be to consider strategies which for the most part are compatible with currently available GP codes. The overall development will be considered in three main levels. The first will involve the use of INR operators to "tunnel" into the solution space in the usual manner. The second level will involve the constant monitoring of the different stages of solution via various quality/convergence/nonlinearity tests. Finally, the last level is an outgrowth of the findings of the second; namely, if one or more of the quality/convergence/nonlinearity tests are violated, various scenarios are then triggered to modify the INR strategy.

Based on the foregoing, the paper will outline in detail the multilevel static solution strategy, the development of the quality/convergence/nonlinearity tests as well as overview the various self-adaptive iterative update procedures. The analytical considerations will be complemented by several numerical experiments which outline the various aspects of the quality/convergence/nonlinearity tests and which demonstrate the self-adaptive strategy.

MULTILEVEL SOLUTION STRATEGY:

OVERVIEW

As noted earlier, unless the proper load incrementation is employed, either poor convergence or out of balance loads are generally encountered. Such anomalous behavior is generic to all nonlinear codes employing non-self-adaptive INR algorithms. In this context, the main thrust of this work is to establish a three level iterative solution strategy involving:

- i) Level 1; Preliminary solution development via the primitive but computationally efficient IMNR algorithm;
- ii) Level 2; Solution monitoring via quality/convergence/nonlinearity tests and;
- iii) Level 3; Self-adaptive update procedures to modify the primitive operator.

Note here computational efficiency is meant to be a measure of the amount of time spent during a cycle of iteration not the overall process.

The main purpose of the first level of the overall strategy is essentially twofold. The first is to generate the most efficient solution if the requisite quality/convergence/nonlinearity criteria are satisfied. If not, the information generated by the IMNR "tunneling" of the solution space can, through the second level tests, trigger the proper third level action.

In terms of the foregoing, it follows that the second level is essentially threefold in nature. The quality check involves monitoring: the rate of convergence; monotonicity; positive, negative and semi-definiteness; etc. The convergence tests check for outright solution failure, and lastly, the nonlinearity tests ascertain the "degree" of nonlinearity excited.

In the third level, the foregoing information is used to trigger various self-adaptive modifications of the IMNR iterative strategy. Namely:

- i) Global stiffness reformation;
- ii) Preferential local reformation and;
- iii) Load increment adjustment.

Such algorithmic adjustments form the heart of the third level of the overall strategy.

INR FAMILY OF STRATEGIES

The overall family of INR strategies can essentially be established by introducing increasingly severe restrictions to the straight methodology. Specifically, starting with the virtual work theorem depicted by [1]

$$\int_R \delta \xi^T \tilde{S} dv = \tilde{Y}^T \tilde{F} \quad (1)$$

the typical FE shape function formulation yields the following nonlinear large deformation field equations [1]

$$\int_R [B^*]^T \tilde{S} dv = \tilde{F} \quad (2)$$

where

$$\delta \xi^T \equiv \frac{1}{2} (\delta u_{i,j} + \delta u_{j,i} + u_{\ell,i} \delta u_{\ell,j} + u_{\ell,j} \delta u_{\ell,i}) \quad (3)$$

$$\tilde{S}^T = (S_{11}, S_{22}, S_{33}, S_{12}, S_{23}, S_{31}) \quad (4)$$

such that ϵ , S , Y and F are, respectively, the strain tensor in vector form, the second Piola Kirchhoff pseudo stress tensor, the nodal displacement vector, and lastly, the nodal force vector.

To solve (2), the Taylor expansion theorem can be used to establish the following tangent stiffness formulation, namely

$$[K_t(Y_{i-1}^l)] \Delta Y_i^l = \Delta F_i \quad (5)$$

where ΔY_i^l denotes the i^{th} nodal displacement iterate associated with the l^{th} load increment. The nodal displacement, tangent stiffness and load imbalance are defined by

$$\tilde{Y}_{i-1}^l = \sum_{k=1}^{l-1} \sum_{j=1}^{I_k} \Delta Y_j^k + \sum_{j=1}^{i-1} \Delta Y_j^l \quad (6)$$

$$[K_t(Y_{i-1}^l)] = \int_R \left\{ [G]^T [\sigma(\tilde{Y}_{i-1}^l)] [G] + [B^*(Y_{i-1}^l)]^T [D_t(Y_{i-1}^l)] [B^*(Y_{i-1}^l)] \right\} dv \quad (7)$$

$$\Delta F_i^l = \tilde{F}^l - \int_R [B^*(Y_{i-1}^l)]^T \sigma(\tilde{Y}_{i-1}^l) dv \quad (8)$$

such that I_k , $[\sigma(Y_{i-1}^l)]$, $[D_t(Y_{i-1}^l)]$ and \tilde{F}^l respectively denote the number of iterations required of k^{th} load step, the initial stress matrix, the tangent material stiffness and the total nodal load after l increments. For the straight INR approach, $[K_t]$ is continuously reformed and inverted. This is obviously quite expensive. In this context, the following versions of the INR algorithm can be established for a specific load increment solution cycle, namely:

- i) Straight INR with constant reformation of tangent stiffness matrix during iteration;
- ii) Intermittent global reformation during iteration;
- iii) Preferential local reformation during iteration;
- iv) BFGS type [3] reformation during iteration;
- v) Classical modified INR procedure wherein stiffness is reformed only at beginning of load step;
- vi) No reformation, just iteration;
- vii) Reformation with no iteration, etc.

As will be seen later, various versions of the foregoing INR family of algorithm are incorporated in the self-adaptive strategy. This will obviously lead to a hierarchy with varying degrees of computation power/efficiency.

QUALITY/CONVERGENCE/NONLINEARITY TESTS

The quality/convergence/nonlinearity tests are the core of the multi-level strategy. Such tests are themselves organized into three main categories, namely:

- i) Classical norm type convergence tests;
- ii) Quality of convergence tests and;
- iii) Degree of nonlinearity tests.

The first group of tests are essentially of the normed type pass or fail variety as typified by:

- a) The out of balance norm test;

$$\|\Delta \mathbf{E}_j^\ell\| / \|\Delta \mathbf{F}_{j-1}^\ell\| < \text{tol} \quad (9)$$

- b) The global displacement norm test;

$$\|\mathbf{Y}_j^\ell\| / \|\mathbf{Y}_{j-1}^\ell\| < \text{tol} \quad (10)$$

The main intent of such tests is essentially to monitor the success or failure of the iterative process. Note, while such tests are efficient and well adapted to this purpose, they cannot be used effectively to forecast potential difficulties until outright failure occurs.

In this context, what is required are so-called quality checks which enable a constant monitoring of the solution so as to determine whether the direction of convergence is proper. This is the purpose of the second stage of checking. Namely, the quality checks test whether the iterative process possesses the requisite: rate; monotonicity; positive, negative and semi definiteness; etc. Once determined, such information is used to trigger the various modifications of the primitive first level IMNR strategy.

Since the paper is mainly concerned with static loading problems, various statements concerning the quality of solution convergence can be made at the outset. For instance, since most static loading is applied in a monotone fashion, it is expected that unless there is overshoot, successive iterated solutions should behave as a monotone, positive, negative or semi definite sequence. Behavior to the contrary obviously represents either overshoot or potential divergence.

Since it is difficult to ascertain the monotonicity and definiteness from either of the normed or vectorial versions of the nodal displacements and forces, alternative field measures must be employed. In this direction, the local (element) and global strain energy stored can serve in such a capacity. This follows from the fact that for monotone loading situations, successive

iterations lead to a monotone positive definite sequence of energy iterates for softening structure. In the case of hardening situations, successive iterates may be nonmonotone for at least the first two iterates. Thereafter, the energy iterates tend to be monotone and negative definite. This process is clearly seen by the normed analogy of the iterative process depicted in Figures 1 and 2.

The incremental iterate energy stored during a given iteration step is essentially the shaded area illustrated in Figure 1. Realizing that the ordinate values of the true solution curve are given by (1), it follows that the incremental energy stored during the k^{ℓ} iteration step of the ℓ^{th} load increment can be approximated by the following inner product, that is

$$\begin{aligned} E_{k+1}^{\ell} &= \frac{1}{2} (\underline{F}_{\sim k}^{\ell} + \underline{F}_{\sim k+1}^{\ell})^T \Delta \underline{Y}_{k+1}^{\ell} = \frac{1}{2} \int_R ([B^*(\underline{Y}_{\sim k}^{\ell})]^T S(\underline{Y}_{\sim k}^{\ell}) + \\ &[B^*(\underline{Y}_{\sim k+1}^{\ell})]^T S(\underline{Y}_{\sim k+1}^{\ell}))^T dv \Delta \underline{Y}_{k+1}^{\ell} \end{aligned} \quad (11)$$

Assuming that a total of K^{ℓ} iteration steps are associated with the ℓ^{th} load-step, then the following expression can be developed for the energy stored, namely:

$$\begin{aligned} E^{\ell} &= \sum_{k=1}^{K^{\ell}-1} E_k^{\ell} = \frac{1}{2} \sum_{k=1}^{K^{\ell}-1} (\underline{F}_{\sim k}^{\ell} + \underline{F}_{\sim k+1}^{\ell})^T \Delta \underline{Y}_{k+1}^{\ell} \\ &= \frac{1}{2} \sum_{k=1}^{K^{\ell}-1} \int_R ([B^*(\underline{Y}_{\sim k}^{\ell})]^T S(\underline{Y}_{\sim k}^{\ell}) + [B^*(\underline{Y}_{\sim k+1}^{\ell})]^T S(\underline{Y}_{\sim k+1}^{\ell}))^T dv \Delta \underline{Y}_{k+1}^{\ell} \end{aligned} \quad (12)$$

Note (12) is essentially a trapezoidal type integration approximation for the area under the hyper-curve defining the solution of the ℓ^{th} loadstep. Now, summing (12) over the entire set of L loadsteps associated with a given problem yields the requisite overall strain energy stored, namely:

$$E_{\text{total}} = \frac{1}{2} \sum_{\ell=1}^L \sum_{k=1}^{K^{\ell}-1} (\underline{F}_{\sim k}^{\ell} + \underline{F}_{\sim k+1}^{\ell})^T \Delta \underline{Y}_{k+1}^{\ell} \quad (13)$$

To obtain the strain energies for say the e^{th} element, (13) must be interpreted from a local point of view. Namely, the requisite partitions of \underline{F}_k^e and $\Delta \underline{Y}_k^e$ must be employed in a partitioned version of (13), that is

$$E_{\text{total}}^e = \frac{1}{2} \sum_{\ell=1}^L \sum_{k=1}^{K^{\ell}-1} (\underline{F}_{\sim k}^{\ell e} + \underline{F}_{\sim k+1}^{\ell e}) \Delta \underline{Y}_{k+1}^{\ell e} \quad (14)$$

where here $\Delta \underline{Y}_{\sim k}^{\ell e}$ and $\underline{F}_{\sim k}^{\ell e}$, are respectively the local and element nodal displace-

ments and forces. Note, due to the form of (14), any form of tangent stiffness type of constitutive law can be accommodated.

In terms of the iteration process associated with softening media, it follows that for convergent situations

$$E_1^\lambda > E_2^\lambda > \dots > E_k^\lambda > E_{k+1}^\lambda \dots > 0 \quad (15)$$

that is, successive iterates are monotone and positive definite. Hence, for softening media, a check of successive iterates for monotone decreasing positive definiteness will establish a measure of the quality of convergence. For the hardening case, the E_k^λ sequence associated with the convergent solution process takes the form:

$$E_2^\lambda < E_3^\lambda < \dots < E_k^\lambda < E_{k+1}^\lambda \dots < 0 < E_1^\lambda \quad (16)$$

As can be seen, for $k>1$, the sequence E_k^λ is monotone increasing but negative definite. In this context, similar to the softening case, a check of the monotone increasing negative definiteness of successive iterates is used as one of the measures of the quality of convergence.

A last but very important way of predicting potential solution difficulties can be achieved by monitoring the degree of nonlinearity excited as the deformation process continues. This can be achieved by selectively checking the changes of curvature of the global and local strain energy space. Such behavior can be ascertained using difference operators to evaluate either the slope, rate of change of slope, or more elaborately, the radius of curvature of the energy space as either a function of the loading parameter or the nodal displacements. An alternative approach would be to locally spline fit the energy-loading parameter space. In this way, the current curvature/slope can be obtained either on a local element or global basis. Such information can be used to initiate changes in load step size as well as to control local and global stiffness reformation.

The importance of such tests follows from the fact that although FE simulations of structures composed of general media undergoing large deflections are inherently nonlinear, the degree of nonlinearity excited varies from point to point as well as from load increment to load increment. As it is possible that large portions of the structure may exhibit basically linear behavior, many general purpose codes allow the user to partition the overall structure into its linear and nonlinear groups. Although this certainly adds to the efficiency of the code, generally such information is not known a priori unless extensive parametric studies have already been performed. In this context, the nonlinearity check will enable the automatic partitioning of the structure by allowing for preferential reformation of the tangent stiffness depending on the amount of local nonlinearity excited.

ADAPTIVE STRATEGY

In the context of the inherent features of the INR family of algorithms, the adaptive strategy incorporates the following procedural options namely:

- i) Tangent stiffness reformation and;
- ii) Load increment adjustment.

Each of these options in turn involves several different levels. For instance, stiffness reformation can be considered in several stages, that is:

- i) Global reformation;
- ii) Preferential local reformation or;
- iii) BFGS [3] reformation.

The adaptive incremental load can also be achieved in several ways namely:

- i) Increment expansion;
- ii) Increment contraction or;
- iii) Corrective incrementation.

As noted earlier, the initiation of either option is dependent on three basic criteria, that is:

- a) Quality of convergence;
- b) Outright failure to converge or;
- c) The degree of nonlinearity excited.

While the reformation option is triggered by the second level tests, the specific adaption triggered is primarily dependent on the degree of nonlinearity excited. Hence, for mildly nonlinear (elastic) situations, the BFGS reformation process is employed. In the case where significant local or global nonlinearity is excited, then either global or preferential reformation is initiated.

As can be seen from the proceeding categories, various types of load incrementation are possible. The overall strategy is a combination of such options. Specifically, when significant solution degradation is monitored by the level two tests, then corrective incrementation is initiated. Namely, negative load incrementation is employed to enable the retracing of a portion of load history wherein a lower order algorithmic strategy yielded poorly converged results.

To strike a balance between solution convergence and economy, the overall

adaptive strategy is centered about a primitive version of the INR algorithm namely the IMNR. Depending on the results of the quality/convergence/nonlinearity tests, the level of the IMNR is either upgraded or lowered by modifying the pattern of stiffness reformation and incrementation. Note, since the main incentive is to achieve a successful solution at least cost, the hierarchy is ordered to first implement increment adjustment and then reformation. As a further move to achieve economy, the global reformation process typically employed at the start of an IMNR increment can be established preferentially depending on the curvature tolerance associated with the global and local non-linearity checks.

Since space is limited, a full description of the various detailed hierarchies must be left to future publications. In this context, for the present purposes, Figure 3 gives a good overview of all the possible flows of control associated with the three-level strategy. As can be seen from this figure, contingent upon the various "flags" generated in the level two tests, the condition code check routine will initiate the actual modification of the INR strategy along the lines outlined in the proceeding discussion.

DISCUSSION

Interestingly, while such factors as geometry, material properties, boundary conditions, etc., all have some effect on the choice of load increment size, once an excessive value has been chosen, typically similar types of solution degradation are encountered when only the primitive non-self-adaptive algorithm is used. Specifically, three basic types of solution pathology tend to occur. These can be categorized by:

- i) Immediate and strong nonmonotonicity;
- ii) Moderate but progressively increasing nonmonotonicity and non-positive definiteness and;
- iii) Mild monotonicity with either very gradual increases or decreases in solution oscillation.

Note, such behavior can be excited either in the first or successive load steps. Figures 4 and 5 give examples of such behavior. While the results illustrated pertain to a rubber sheet, similar results were obtained for elastic/plastic media as well as for different geometries and boundary conditions.

The solution failure depicted in Figure 5 is typical of those that usually arise. Specifically, as can be seen, for the given load increment excellent convergence is obtained in the first step. In the second, a mild form of non-monotonicity and nonpositive definiteness is encountered. Finally, in the third step, strong and progressively increasing nonpositive definiteness is encountered. Solution failure is finally initiated by out of balance loads. This scenario is typical of excessive load incrementation. Note, as can be seen from these results, the onset of such behavior is signalled by the initiation of nonmonotonicity or incorrect definiteness. By studying the behavior

of local element energies, additional insights are obtained. For the problems illustrated in Figures 4 and 5, the solution degradation is initially localized but gradually spreads to the entire structure as the iteration process continues. Employing the self-adaptive strategy to the foregoing problems caused the second level monotonicity tests to trigger automatic increment adjustment and preferential stiffness reformation. This led to the generation of the correct solution. The overall strategy was tested on several nonlinear problems which exhibited pathological behavior for given load increment choices. The types of problems considered combined varying degrees of kinematic, kinetic and material nonlinearity. In each case barring possible bifurcations, the level two tests were able to automatically initiate the requisite corrective self adaptions to enable successful solutions. The main problem encountered with the concept of self-adaptive strategies arises from the fact that some engineering insight must be practiced in order to cut down overall running times. Otherwise, excessive execution times are encountered as the adaptive strategy shifts gears to adjust for improper incrementation.

REFERENCES

1. Zienkiewicz, O. C., "The Finite Element Method", McGraw Hill Co. New York, 1978.
2. Chang, T. Y. and Padovan, J., "General Purpose Finite Element Programs," Structural Mechanics Software Series, Vol. III, Nicholas Parrone and Walter D. Pilkey, eds., Univ. Press of Va., 1980.
3. Strang, G., "Numerical Computations in Nonlinear Mechanics", ASME Paper No. 79-PVP-114.

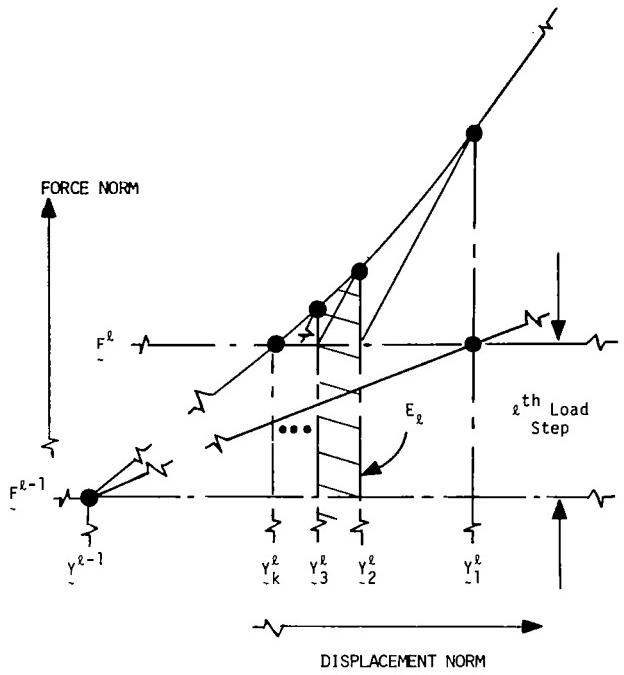


Figure 1.- Iteration process for hardening problem.

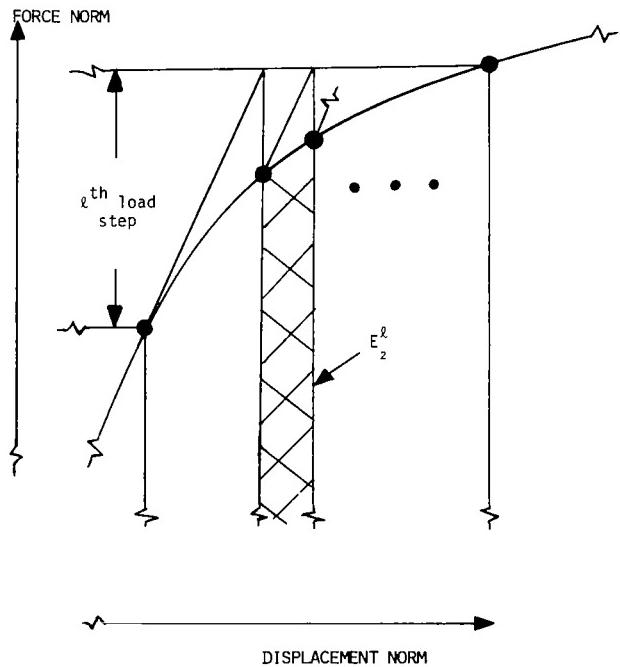


Figure 2.- Iteration process for softening problem.

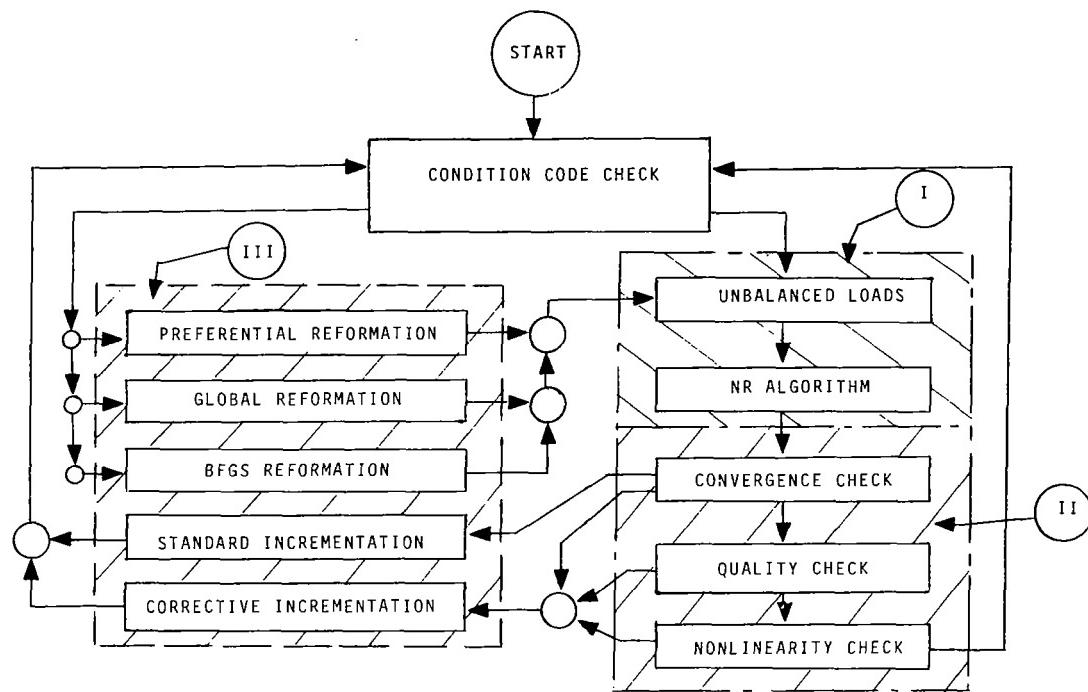


Figure 3.- Overall flow of control of three-level self-adaptive strategy.

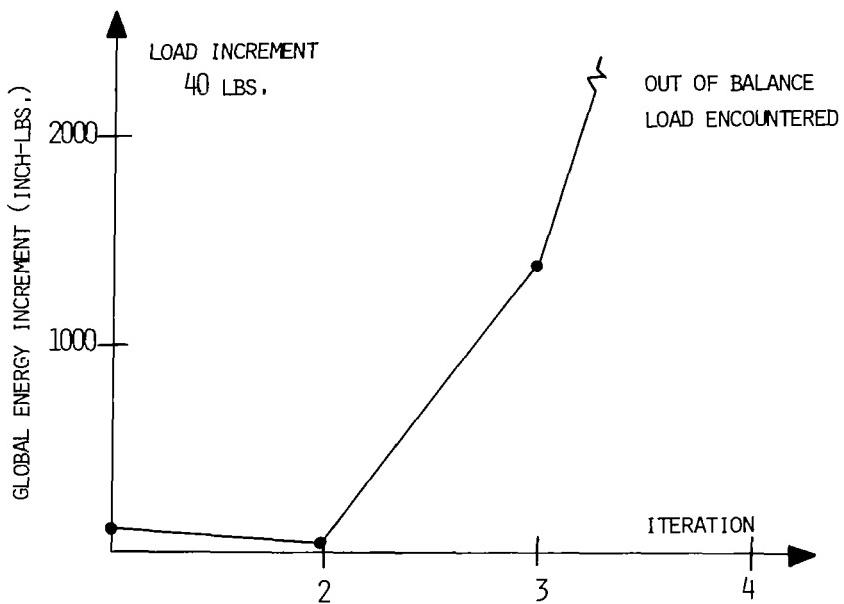


Figure 4.- Global energy increment of rubber sheet (1st load step).

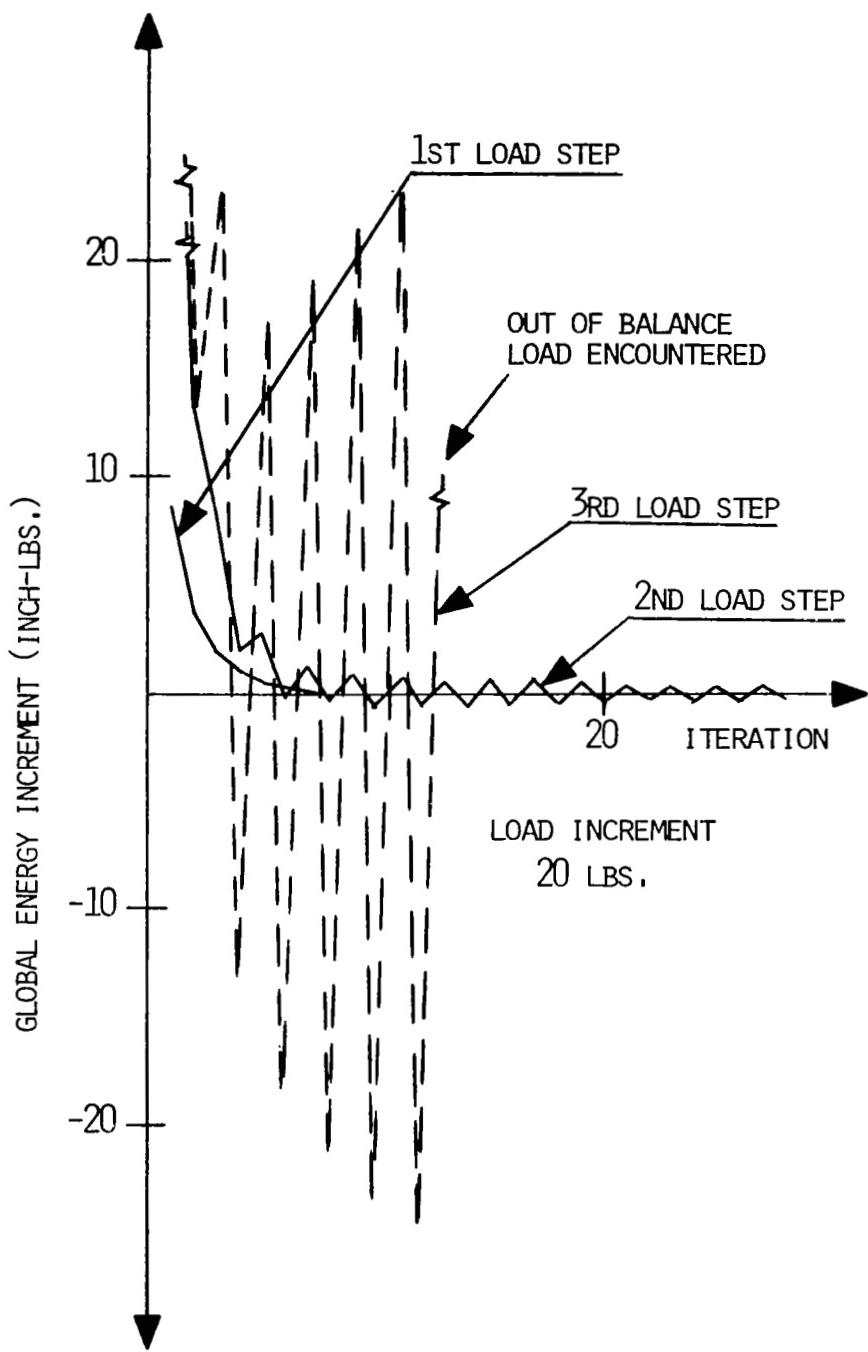


Figure 5.- Global energy increment of rubber sheet
(1st, 2nd, 3rd load steps).